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High orders of the perturbation theory for hydrogen atom in magnetic field

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Abstract

The states of hydrogen atom with principal quantum number $n \leq 3$ and zero magnetic quantum number in constant homogeneous magnetic field \mathcal{H} are considered. The coefficients of energy eigenvalues expansion up to 75th order in powers of \mathcal{H}^2 are obtained for these states. The series for energy eigenvalues and wave functions are summed up to \mathcal{H} values of the order of atomic magnetic field. The calculations are based on generalization of the moment method, which may be used in other cases of the hydrogen atom perturbation by a polynomial in coordinates potential.

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1. INTRODUCTION

A new aspect of the problem of hydrogen atom in constant electric (\mathcal{E}) and magnetic (\mathcal{H}) external fields was observed recently. It was found [1], that the asymptotic of the perturbation series in powers of \mathcal{E} considerably changes at some \mathcal{H} values. This change is related with complex solutions of classical equations of motion, previously not taken into account. A look at this phenomenon from the expansion in powers of \mathcal{H} point of view could be useful. Our work is aimed just in this direction. An effective method for building the perturbation series is offered and the asymptotic of this series for the Zeeman effect is discussed here.

The moment method for high orders of the perturbation theory evaluation, possessing additional possibilities as compared with the other known recurrent methods, was introduced in Ref. [2]. It was described as an expedient for dimensional expansion investigation — in a problem leading to effective isotropic anharmonic oscillator. Then it was applied to dimensional expansion for three body problem [3], where the effective anharmonic oscillator is anisotropic.

We turn our attention to the fact, that the perturbation of the hydrogen atom by a potential of polynomial form is also convenient to investigate by the moment method. The constant homogeneous electric and magnetic fields are referred just to this kind of perturbations. The advantages of the moment method are clearly seen in the Zeeman effect problem. High orders of the perturbation theory (PT) using different approaches were studied in Refs. [4-6]. The method, based on the group theory was applied. 36 coefficients of the hydrogen's ground state energy expansion in powers of \mathcal{H}^2 were published in Ref. [6]. For excited states Zeeman's PT coefficients not higher than of the third order in \mathcal{H}^2 are given in Refs. [7-10]. The variables in the Schrödinger equation for the Zeeman effect can not be separated and it makes computation of higher PT orders more difficult. The moment method does not require variables separation. Besides, as it will be shown here, this method can be applied to degenerate states. Obviously this possibility is essential for most of the hydrogen atom states.

Apparently the logarithmic perturbation theory (LPT) was most frequently used for recurrent evaluation of PT coefficients up to now [11-15]. Owing to its simple algebraic structure, LPT allowed to compute the highest orders corrections for some cases. Thus, for the Stark shift of the hydrogen ground state 160 orders of PT were obtained this way [16]. But LPT is not free from restrictions. Even one node of the wave function leads to considerable more complicated computation procedure [17]. Much more complicated LPT looks in problems, where variables can not be separated. Without variables separation only a few initial PT orders were computed with the help of LPT for the hydrogen atom in electric and magnetic fields [9,10,14].

It is also worth mentioning here the old PT version, based on the generalized virial and Hellmann–Feynman theorems, which anticipated the modern moment method. In Refs. [18,19] recurrence relations were written for problems with spherical symmetry, allowing to compute energy eigenvalues corrections for states with nodes in as simple way as for nodeless states. But the moments introduced in these papers were diagonal ones and that is why the region of applicability of

the method is restricted. For instance, in this formalism it is impossible to obtain the corresponding wave function.

The recurrence relations of the Ader moment method will be obtained below. Two examples illustrate their applications: one is referred to non-degenerate state and the other to the case of degeneracy. Then the asymptotic of the numerically obtained energy expansion coefficients is considered and the results of summation of perturbation series are given. It will be shown on example of the ground state, how the wave function of the perturbed hydrogen atom can be obtained within the moment method.

2. MAIN RECURRENCE RELATION

Consider the state of the hydrogen atom $|\psi_0\rangle = |n, l\rangle$ with principal quantum number n , angular momentum l and zero projection of the angular momentum $m = 0$, perturbed by strong magnetic field $\mathcal{H} = \mathcal{H}_z$. Let us write expansions of the energy eigenvalue and the wave function of this state in the form

$$E = \sum_{k=0}^{\infty} E_k \gamma^{2k}, \quad \psi(\vec{r}) = \sum_{k=0}^{\infty} \psi_k(\vec{r}) \gamma^{2k}, \quad (1)$$

$$\gamma = n^3 \mathcal{H} / \mathcal{H}_0, \quad \mathcal{H}_0 = e^3 m^2 c / \hbar^3 = 2.35 \times 10^9 G.$$

Here ψ_k is the correction of the order k to the Coulomb wave function, which satisfies the inhomogeneous equation

$$(\hat{H}_0 - E_0)\psi_k = -\hat{H}_1\psi_{k-1} + \sum_{j=1}^k E_j \psi_{k-j}, \quad (2)$$

where

$$\hat{H}_0 = -\frac{1}{2}\nabla^2 - \frac{1}{r}, \quad \hat{H}_1 = \frac{1}{8}(r^2 - z^2).$$

(We use atomic units.) To change the differential equation by an algebraic one we introduce the moments of the order k

$$P_{\sigma\nu}^k = \langle \tilde{\psi}_0 | r^{\sigma-\nu} z^\nu | \psi_k \rangle, \quad (3)$$

where

$$|\tilde{\psi}_0\rangle = C e^{-r/n}, \quad \sigma \text{ and } \nu \text{ are integer.}$$

In this definition $|\tilde{\psi}_0\rangle$ contains only exponential factor of the unperturbed wave function, bearing its scale and having no nodes. (Note, that the common normalization factor of all moments can be chosen arbitrary.) Just as it was done in Ref. [2], multiply Eq. (2) from the left by $\langle \tilde{\psi}_0 | r^{\sigma-\nu} z^\nu$ and use the possibility for the hamiltonian to act to the left, on explicitly known functions. This way the recurrence relation for moments of the order k results:

$$\frac{(\sigma - \nu)(\sigma + \nu + 1)}{2} P_{\sigma-2, \nu}^k + \frac{\nu(\nu - 1)}{2} P_{\sigma-2, \nu-2}^k - \frac{\sigma + 1 - n}{n} P_{\sigma-1, \nu}^k + P_{\sigma\nu}^0 E_k = R_{\sigma\nu}^{k-1}, \quad (4)$$

where

$$R_{\sigma\nu}^{k-1} \equiv \frac{1}{8}(P_{\sigma+2,\nu}^{k-1} - P_{\sigma+2,\nu+2}^{k-1}) - \sum_{j=1}^{k-1} E_j P_{\sigma\nu}^{k-j} .$$

The right-hand side of Eq. (4) contains moments only of preceding orders. The E_k coefficient, which we call the hyper-susceptibility of the order k , can also be expressed through the preceding orders moments. This expression follows from (4) and will be written down below, separately for each of the cases under investigation.

Quite similar it is possible to consider another perturbation of the same state, if this perturbation has the form of a polynomial in r and z . It is enough to change only the right-hand side of Eq. (4) for this aim. The expression in brackets in the right-hand side, representing the magnetic field contribution, should be replaced by another function of the preceding orders moments, created by the new perturbation.

The succession of the based on relation (4) computations becomes more lucid if one represents on a plot the lattice of points with integer coordinates of columns σ and rows ν . The indices of moments, necessary to compute energy and wave function corrections, are placed on this lattice in the sector $\sigma \geq \nu - 1$, $\nu \geq 0$. In the general case Eq. (4) relates moments of the order k , indices of which are located in the vertices of a rectangular triangle (see examples in Fig. 1). When one vertex appears to be on the line $\sigma = \nu - 1$ and another one is outside the above indicated sector, the triangle (example *A*) transforms into segment (example *B*), and Eq. (4) turns into relation between two moments from different rows. Equation (4) relates moments in pairs also along each of the lines with $\nu = 0$ and $\nu = 1$ (examples *C* and *D*). At $k = 0$, as the direct integration indicates, among the moments $\langle \tilde{\psi}_0 | r^{\sigma-\nu} z^\nu | n, l \rangle$ are equal to zero those, for which $l - 1 \leq \sigma < n - 2$. If the perturbation is even, as in the case of the Zeeman effect, all corrections to the wave function have the same parity. Therefore, in all PT orders the moments with odd sum $\nu + l$ vanish.

3. ISOLATED STATES

Magnetic field does not mix states with different parities, therefore besides the ground state, $2s$ -, $2p$ - and $3p$ -states should also be considered as non-degenerate. Let us show, how the moment method works in the last case. Only the moments with odd ν values can be different from zero. In initial PT order

$$P_{\sigma, 2\alpha+1}^0 = -\frac{\sigma(\sigma+3)!}{18(2\alpha+3)} \left(\frac{3}{2}\right)^\sigma, \quad \alpha \text{ is integer} . \quad (5)$$

For all following orders an additional requirement is introduced: corrections to the function $|\psi_0\rangle$ should be orthogonal to the function $|\psi_0\rangle$ itself, i.e. $\langle \psi_0 | \psi_k \rangle = \delta_{0,k}$. This condition is the routine element of the Brillouin-Wigner perturbation theory (see, e.g. [20]). It was used in Ref. [2]. In the case of $3p$ -state it takes the form of the following additional relation between the moments

$$P_{11}^k - \frac{1}{6} P_{21}^k = \delta_{0,k} . \quad (6)$$

To obtain an expression for E_k , we substitute into recurrence relation (4) first $\nu = 1$, $\sigma = 1$, then $\nu = 1$, $\sigma = 2$. The solution of the obtained system of two linear equations is

$$E_k = R_{11}^{k-1} - \frac{1}{6}R_{21}^{k-1} = \frac{1}{8}(P_{31}^{k-1} - P_{33}^{k-1}) - \frac{1}{48}(P_{41}^{k-1} - P_{43}^{k-1}) , \quad (7)$$

$$P_{01}^k = 5R_{11}^{k-1} - \frac{1}{3}R_{21}^{k-1} . \quad (8)$$

The sum, containing hyper-susceptibilities of preceding orders, dropped out of the final expression for E_k owing to orthogonality condition (6).

Equations (4), (6) and (7) form the closed system of recurrence relations. In each order $k \geq 1$ the sequence of computations is arranged as follows. First, the coefficient E_k is evaluated with the help of (7). On the next step $\nu = 1$ and $\sigma = 3$ are substituted into recurrence relation (4). In this case together with orthogonality condition (6) it forms a system of equations from which initial elements of the row of moments with $\nu = 1$ are obtained:

$$P_{11}^k = \frac{1}{3}(R_{31}^{k-1} - P_{31}^0 E_k) = \frac{1}{6}P_{21}^k .$$

Successively increasing σ by one, it is not difficult to come to the necessary boundary moment of this row. Substituting then in Eq. (4) $\nu = 3$ and $\sigma = 3$, we get the initial moment of the next row

$$P_{33}^k = 3(3P_{11}^k - R_{33}^{k-1} + P_{33}^0 E_k)$$

and so on.

The boundary moments, i.e. the moments with the highest for the given order k indices σ and ν values are determined by the following conditions. To compute the hyper-susceptibility of high order K the following moments are required: $P_{\sigma\nu}^1$ from the region $\nu - 1 \leq \sigma \leq 3K$, $0 \leq \nu \leq 2K$, then $P_{\sigma\nu}^2$ from the region $\nu - 1 \leq \sigma \leq 3K - 3$, $0 \leq \nu \leq 2K - 2$ and so on. The computation of E_k coefficients for the other isolated states goes a bit more simple.

4. DEGENERATE STATES IN THE MOMENT METHOD

We consider as an example a pair of splitted by the magnetic field states $|3s\rangle$ and $|3d\rangle$. Taking into account degeneracy and using the functions

$$|\psi_0\rangle = \cos \alpha |3s\rangle + \sin \alpha |3d\rangle , \quad |\tilde{\psi}_0\rangle \sim e^{-r/3} ,$$

it is not difficult to obtain the zero order moments

$$P_{\sigma, 2\alpha}^0 = \frac{(\sigma + 2)!}{54(2\alpha + 1)} \left(\frac{3}{2}\right)^\sigma \left(\sigma(\sigma + 1) - \frac{\alpha(\sigma + 3)(\sigma + 4)}{2\alpha + 3} \xi \right) , \quad (9)$$

where

$$\xi = \sqrt{2} \operatorname{tg} \alpha .$$

The moments in odd rows are equal to zero in all PT orders, $P_{\sigma,2\pi+1}^k = 0$. The orthogonality condition $\langle \psi_0 | \psi_k \rangle = \delta_{0,k}$ is equivalent to the following relation between the moments:

$$12P_{10}^k - \frac{1}{3}(4 + \xi)P_{20}^k + \xi P_{22}^k = 18P_{00}^k, \quad k \geq 1. \quad (10)$$

There are two independent ways for expressing hyper-susceptibility E_k through preceding orders moments.

a) Equation (4) at $\nu = 0$ and $\sigma = 0$ determines the moment $P_{-1,0}^k$, which is used on the next step in the system of linear equations. Note that E_k coefficient drops out of Eq. (4) as a consequence of $P_{00}^0 = 0$ equality. The system of equations, containing E_k arises if one put in Eq. (4) first $\nu = 0$, $\sigma = 1$, and then $\nu = 0$, $\sigma = 2$. Its solution is

$$E_k^{(a)} = \frac{9}{2}R_{00}^{k-1} - 3R_{10}^{k-1} + \frac{1}{3}R_{20}^{k-1}, \quad (11a)$$

$$P_{00}^k = -9R_{00}^{k-1} + 6R_{10}^{k-1} - \frac{1}{3}R_{20}^{k-1}. \quad (12)$$

The obtained as a by-product moment P_{00}^k is substituted into the right-hand side of orthogonality condition (10).

b) Substituting into Eq. (4) $\nu = 2$ and $\sigma = 2$ together with the obtained P_{00}^k value, we get the second independent expression for E_k

$$E_k^{(b)} = \frac{1}{2}(9R_{00}^{k-1} - 6R_{10}^{k-1} + \frac{1}{3}R_{20}^{k-1} + R_{22}^{k-1}). \quad (11b)$$

Equations (11a) and (11b) result in single magnetic susceptibility E_1 value at two ξ values:

$$\xi = \xi_{1,2} = \frac{-13 \pm 3\sqrt{41}}{10} \quad (13)$$

It is a natural result, which in Rayleigh-Schrödinger PT follows from the secular equation. In what follows the notation $3s$ is kept for the state with small admixture of d -wave and $\xi = \xi_1 = (3\sqrt{41} - 13)/10$, and $3d$ denotes the orthogonal to this state combination of s - and d -waves. In the following approximations the unambiguity condition, applied to hyper-susceptibility of $(k+1)$ th order, $E_{k+1}^{(a)} = E_{k+1}^{(b)}$ is equivalent to relation between seven unknown moments of the order k :

$$\begin{aligned} \xi[9(P_{20}^k - P_{22}^k) - 6(P_{30}^k - P_{32}^k)] - \frac{1}{3}(1 - 2\xi)P_{40}^k + \frac{2}{3}(1 + \xi)P_{42}^k - P_{44}^k = \\ 8[\xi(9S_{00}^k - 6S_{10}^k) - \frac{1}{3}(1 - 2\xi)S_{20}^k + S_{22}^k]. \end{aligned} \quad (14)$$

Here $S_{\sigma\nu}^k = \sum_{j=1}^k E_j P_{\sigma\nu}^{k-j}$ and $\xi = \xi_{1,2}$. One more constraint on the moments is orthogonality condition (10). To obtain a closed system, Eqs. (10) and (14) should be supplemented by seven equations, following from recurrence relation (4). The set of unknown variables includes $P_{10}^k, P_{20}^k, P_{30}^k, P_{40}^k, P_{22}^k, P_{32}^k, P_{42}^k, P_{34}^k, P_{44}^k$. It is enough to determine only two moments P_{10}^k and P_{22}^k

from the system of nine equations. Then, with the help of already known moments and relation (4) it is not difficult to compute successively all necessary moments of the given order, passing line by line the lattice of indices, like in the case of $3p$ -state.

Quite similar, it is possible to accomplish the computation for a state with arbitrary n value and zero projection of angular momentum. The unperturbed wave function has definite parity and contains g degenerate in energy terms. Therefore $g - 1$ independent mixing parameters explicitly enter the zero order moments. There are two groups of moments in every order $k \geq 1$. Recurrence relation (4) connects the moments $P_{\sigma\nu}^k$ with $\sigma < n - 2$ and separately the moments of the same order but with $\sigma \geq n - 2$. Moments from different groups are connected by recurrence relation only through the moments of preceding orders.

To obtain all independent expressions for E_k , one should substitute into recurrence relation (4) the successively increasing ν values of the given parity and corresponding set of σ values:

$$0 \leq \nu \leq \sigma \leq n - 1 .$$

At every ν value the unambiguously solvable system of equations is obtained. Its solution contains independent expression for E_k and a set of moments of the order k , to be substituted in analogous system at the next ν value. Thus, g independent expressions for E_k in terms of the preceding orders moments result. The unambiguity condition of E_1 determines $g - 1$ mixing coefficients. The unambiguity condition of E_{k+1} at $k \geq 1$ allows to express the moments $P_{\sigma\nu}^k$ from the domain $\sigma \geq n - 2$ through preceding orders moments. The equations expressing the unambiguity of E_{k+1} are supplemented by orthogonality condition $\langle \psi_0 | \psi_k \rangle = 0$ and by necessary number of equations, obtained from recurrence relation (4), to close the system.

5. RESULTS

Energy eigenvalues

For all levels with $n \leq 3$ and $m = 0$ with the help of the moment method we have obtained Zeeman's hyper-susceptibilities E_k up to 75th order, see Table 1. All computations were carried out with 32 decimal digits. Complete agreement is observed with the results of Ref. [8] and Ref. [7], containing first five coefficients E_k for the ground state and three initial coefficients for both $2s$ - and $2p$ -states in the form of rational fractions. In Ref. [9] a difference was detected between the obtained in this work expression for E_2 coefficient and its value at $l = 1$ in Ref. [7]. This deviation is confirmed. As it follows from expression of Ref. [9], $E_2^{(2p)} = -45.556$, but our result is $E_2^{(2p)} = -42$ in agreement with [7].

Energy eigenvalues $E(\gamma)$ of six states, obtained by corresponding power series (PS) summation with the help of Padé approximants $[L/L](\gamma^2)$ and $[L/L - 1](\gamma^2)$ are shown in Figs. 2a-2c. These figures represent also the region of convergence of Padé approximants. Without expansion in \mathcal{H}^2 , by means of the splines method, which is one of modifications of the variational method, energy

eigenvalues of states under consideration were computed for some \mathcal{H} values in Ref. [21]. They are also indicated in Figs. 2a-2c. Reference [21] has the best precision among all non-perturbative calculations and contains a comparison of a large number of previous computations. The precision of PS summation with the help of Padé approximants is high enough. At $\gamma \approx 1$ for $2s$ - and $3p$ -states three or four stable digits of energy eigenvalue are established, and at least two decimal digits for energies of the other states are obtained. Results of PT series summation together with some results of Ref. [21] are represented in Table 2. This table also illustrates convergence of Padé approximants we used. The convergence is sharply increased with γ decreasing, and at $\gamma < 0.3$ the precision of PS sum exceeds the precision of variational calculations [21].

The PT coefficients E_k approach, as the order increases, to the asymptotic, the leading term of which for the Zeeman effect is [4,5]:

$$\tilde{E}_k = (-1)^{k+1} \frac{D_{nl}}{\pi^{2n+1/2}} \left(\frac{n^2}{\pi} \right)^{2k} \Gamma(2k + 2n - 1 + \frac{(-1)^l}{2}) . \quad (15)$$

For the levels under consideration

$$D_{1s} = 32 , \quad D_{2s} = 128 , \quad D_{2p} = 64 ,$$

$$D_{3s} = \frac{2^{15}}{3^4} \left(\alpha_1 - \frac{\alpha_2}{2\sqrt{2}} \right)^2 , \quad D_{3d} = \frac{2^{15}}{3^4} \left(\alpha_2 + \frac{\alpha_1}{2\sqrt{2}} \right)^2 ,$$

where

$$\alpha_1 = - \left(\frac{1}{2} + \frac{13}{6\sqrt{41}} \right)^{1/2} , \quad \alpha_2 = \left(\frac{1}{2} - \frac{13}{6\sqrt{41}} \right)^{1/2} .$$

This result was obtained by the method introduced by Bender and Wu [22]. First, the penetrability of the barrier at imaginary magnetic field value was computed in quasiclassical approximation, then the dispersion relation in \mathcal{H}^2 was applied. Strictly speaking, according to the conditions of Ref. [5], expression (15) is not referred to the case of $3p$ -state. But it is reasonable to suppose that formula (15) describes all six discussed here states with coefficient D_{3p} fitted by comparing E_k and \tilde{E}_k of sufficiently high orders. The result is $D_{3p} = 2^{13}/3^3$. The approach of exact coefficients E_k to asymptotic (15) is illustrated by Fig. 3.

In Refs. [4,5] the corrections to the asymptotic \tilde{E}_k were obtained for some states, among which $2s$ -, $2p$ - and $3p$ -states were absent. Writing the corrections as

$$\frac{E_k}{\tilde{E}_k} = c_0 + \frac{c_1}{2k} + \frac{c_2}{(2k)^2} + \dots , \quad (16)$$

it is not difficult, following the method of Ref. [22], to obtain c_i coefficients for all missing in [4,5] states, see Table 3. As the number of c_i coefficients included in Eq. (16) is increased, the precision of their determination increases as well.

For $3p$ -state this stability of the power correction coefficients confirms that the leading term \tilde{E}_k of the asymptotic is determined correctly. Note, that due to dispersion relation in \mathcal{H}^2 [5] coefficients c_i are related with the corrections to quasiclassical approximation for the barrier penetrability at

$\mathcal{H}^2 < 0$. The straightforward computation of quasiclassical corrections is a complicated enough problem.

Wave functions

By analogy with the anharmonic oscillator [2] case, the correction $|\psi_k\rangle$ to the Coulomb wave function has the form of a polynomial in r and $\cos\theta$, multiplied by $|\tilde{\psi}_0\rangle$. The perturbation is a polynomial and the operator in the left-hand side of Eq. (2) does not change the suggested structure of $|\psi_k\rangle$. For the ground state

$$|\psi_k\rangle = \left(\sum_{j=0}^k \sum_{i=2j}^{3k} a_{ij}^{(k)} r^i \cos^{2j} \theta \right) |\tilde{\psi}_0\rangle \equiv \left(\sum_{j=0}^k \sum_{i=2j}^{3k} a_{ij}^{(k)} r^{i-2j} z^{2j} \right) |\tilde{\psi}_0\rangle . \quad (17)$$

A remark about the origin of the summation boundaries should be done. The θ dependence is introduced only by the expression $r^2 \cos^2 \theta$, contained in \hat{H}_1 , therefore minimal power of radius in the internal sum of expression (17) coincides with the power of $\cos\theta$, and the highest power of $\cos^2\theta$ coincides with PT order. It is possible to check with the help of Eq. (2) that the highest power of radius in $|\psi_k\rangle$ is bigger by three than that in $|\psi_{k-1}\rangle$. A system of linear equations determining coefficients $a_{ij}^{(k)}$ follows from (17) and looks like

$$\sum_{j=0}^k \sum_{i=2j}^{3k} P_{i+\alpha, j+\beta}^0 a_{ij}^{(k)} = P_{\alpha\beta}^k , \quad (18)$$

$$2\beta \leq \alpha \leq 3k , \quad 0 \leq \beta \leq k .$$

In place of the indicated α and β values one can choose another their set, resulting in $(2k+1)(k+1)$ independent equations. This possibility is useful to check the precision of computations. We checked also the orthogonality of the obtained corrections (17) to the function $|\psi_0\rangle$. In our computation the orthogonality condition was preserved with a reasonable precision up to 18th PT order. Corrections to the wave functions up to second order are given in Ref. [7]. By comparing this work and our one the single point of deviation was observed. The sign at the $r^3\gamma^2$ term in Ref. [7] is erroneous and as a result the first order correction is not orthogonal to unperturbed wave function in work [7].

Within the moment method we have computed $|\psi(0)|^2$ values by summing with the help of Padé approximants the PT series for the normalization factor and for the wave function itself. Results are represented in Fig. 4. One can see that 18 PT orders allow to advance up to $\gamma \approx 0.4$. Besides, there is an agreement with Ref. [23], where the wave function of the ground state was computed by a different method.

6. CONCLUSIONS

A good agreement between energy eigenvalues obtained by PT series summation and the corresponding results of independent variational calculations provides a twofold verification. First, it

is confirmed that the computed PT coefficients are correct. Then, the absence of non-perturbative contributions to energy eigenvalues is indicated (the summation method is chosen correctly).

Our investigation demonstrates the high efficiency of the Ader moment method. Let us stress once more the properties of the method which allowed to obtain the high PT orders for the Zeeman effect. These properties could be useful for solving some other problems of the perturbation theory.

- The simple enough recurrence relations are obtained without variables separation in the initial equation. With their aid the corrections computation is reduced to purely algebraic procedure.

- The nodes of the wave function are not shown explicitly and do not complicate the computations. As a consequence the excited states can be considered.

- The level degeneracy, as was demonstrated above, does not restrict application of the moment method, but it leads to more complicated sequence of operations when solving the recurrence relations.

- Besides, the set of moments used for hyper-susceptibilities determination contains information about the wave function. Corrections to Coulomb wave function, just as corrections to energy eigenvalues, follow from purely algebraic procedure.

As it was already mentioned, application of the moment method to the hydrogen atom is not restricted by the Zeeman effect case. Any perturbation of the kind $V(r) = \sum b_{ij} r^{i-j} z^j$ leads to recurrence relation (4) with an obvious simple modification of the right-hand side. For example, this way it is possible to take into account the joint influence of external electric and magnetic fields, homogeneous or consisting of finite number of multipoles.

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Table 1. Hyper-susceptibilities of hydrogen atom in magnetic field.

<i>1s – state</i>		<i>2s – state</i>
<i>k</i>	<i>E_k</i>	<i>E_k</i>
1	$+2.500000000000000000000000000000 \times 10^{-1}$	$+3.500000000000000000000000000000 \times 10^0$
2	$-2.760416666666666666666666666667 \times 10^{-1}$	$-1.593333333333333333333333333333 \times 10^2$
3	$+1.211154513888888888888888888889 \times 10^0$	$+2.250844444444444444444444444444 \times 10^4$
4	$-9.75540590639467592592592592593 \times 10^0$	$-5.51663442962962962962962962963 \times 10^6$
5	$+1.17863024612238377700617283951 \times 10^2$	$+1.88165092810271604938271604938 \times 10^9$
6	$-1.95927276058352435076678240741 \times 10^3$	$-8.20439178651205530864197530864 \times 10^{11}$
7	$+4.27486169952196866486628589997 \times 10^4$	$+4.38959673572860094025228856975 \times 10^{14}$
8	$-1.18693528256085740621952195187 \times 10^6$	$-2.81689767929056062290444312309 \times 10^{17}$
9	$+4.09726018688028425780092822833 \times 10^7$	$+2.13733235781748489849361215413 \times 10^{20}$
10	$-1.72515623494757933487367089115 \times 10^9$	$-1.89790071689337590593564645501 \times 10^{23}$
11	$+8.71666539327097376193289896759 \times 10^{10}$	$+1.95582352962753949948044058249 \times 10^{26}$
12	$-5.21094093401193811088710286758 \times 10^{12}$	$-2.32142997906702906114575376593 \times 10^{29}$
13	$+3.64053240123290947096878491058 \times 10^{14}$	$+3.15101443471988021776783108519 \times 10^{32}$
14	$-2.94037039347649323969534446706 \times 10^{16}$	$-4.85797163582017764548476077630 \times 10^{35}$
15	$+2.71957243076911667415082196285 \times 10^{18}$	$+8.45204454588950406643659448685 \times 10^{38}$
20	$-1.08008064080683361642422438535 \times 10^{29}$	$-6.77777320558482045836185652856 \times 10^{55}$
30	$-1.60767231445546160409172754060 \times 10^{53}$	$-2.69333119877780660677693447444 \times 10^{92}$
40	$-1.86009993885524622493595668510 \times 10^{80}$	$-6.32192703798840441487069765398 \times 10^{131}$
50	$-3.13170157718318015959704309179 \times 10^{109}$	$-1.86940626135923124849582995810 \times 10^{173}$
60	$-2.82752607152079516815460149212 \times 10^{140}$	$-2.71176213794760523959296668884 \times 10^{216}$
70	$-7.04995099684986774958800182910 \times 10^{172}$	$-1.02247285421591824260835479011 \times 10^{261}$
75	$+3.31500360451477843327480892738 \times 10^{189}$	$+5.81143908209506920438376327293 \times 10^{283}$

Table 1. Continuation A.

<i>2p – state</i>		<i>3s – state</i>
<i>k</i>	<i>E_k</i>	<i>E_k</i>
1	$+1.500000000000000000000000000000 \times 10^0$	$+1.95785147671119547722992448839 \times 10^1$
2	$-4.200000000000000000000000000000 \times 10^1$	$-7.99255848864256699334910438169 \times 10^3$
3	$+4.240000000000000000000000000000 \times 10^3$	$+9.86542519182491373199618234956 \times 10^6$
4	$-7.43649066666666666666666666667 \times 10^5$	$-2.09268850909736967372029449066 \times 10^{10}$
5	$+1.87097828977777777777777777778 \times 10^8$	$+5.88259296456916749962643192656 \times 10^{13}$
6	$-6.23210518955750264550264550265 \times 10^{10}$	$-2.03491551010345668150921550764 \times 10^{17}$
7	$+2.63615589562176770773494583018 \times 10^{13}$	$+8.31244877905745777735770437889 \times 10^{20}$
8	$-1.38041101245356842308845936964 \times 10^{16}$	$-3.91936927735269422610169429796 \times 10^{24}$
9	$+8.78777021937730413143094721050 \times 10^{18}$	$+2.10554214073622864491511736652 \times 10^{28}$
10	$-6.70289485780879092143754218449 \times 10^{21}$	$-1.27856250168620586782771927856 \times 10^{32}$
11	$+6.04903613875484403654574962209 \times 10^{24}$	$+8.73019078199070904206045207631 \times 10^{35}$
12	$-6.38629370869963249560760013166 \times 10^{27}$	$-6.67712550914959188602686231758 \times 10^{39}$
13	$+7.80769206270237413951487473753 \times 10^{30}$	$+5.70134624264532995993336408500 \times 10^{43}$
14	$-1.09524180989414207944239838172 \times 10^{34}$	$-5.41744227892988968803716808669 \times 10^{47}$
15	$+1.74827746288164542821561289029 \times 10^{37}$	$+5.70970876646976596904731808022 \times 10^{51}$
20	$-9.93004508733968922803863745812 \times 10^{53}$	$-3.11636589919914001005211784216 \times 10^{72}$
30	$-2.49139318960793926600959408638 \times 10^{90}$	$-3.53759135634213416803068610350 \times 10^{116}$
40	$-4.27118446981052432109181315161 \times 10^{129}$	$-1.74975503131501618694229226731 \times 10^{163}$
50	$-9.94612680182593582345101783873 \times 10^{170}$	$-9.32290913905465430025588878862 \times 10^{211}$
60	$-1.18983403811968620569412506832 \times 10^{214}$	$-2.21489826289171591863053880143 \times 10^{262}$
70	$-3.81690935673691049129436112647 \times 10^{258}$	$-1.28257798832278036045229086676 \times 10^{314}$
75	$+2.01879251467438954569448392302 \times 10^{281}$	$+2.80538297459908381755301158907 \times 10^{340}$

Table 1. Continuation B.

<i>3p – state</i>		<i>3d – state</i>
<i>k</i>	<i>E_k</i>	<i>E_k</i>
1	$+9.000000000000000000000000000000 \times 10^0$	$+5.17148523288804522770075511605 \times 10^0$
2	$-3.531093750000000000000000000000 \times 10^3$	$-1.01742588635743300665089561831 \times 10^3$
3	$+3.448138675781250000000000000000 \times 10^6$	$+6.44144210626019957028207894340 \times 10^5$
4	$-5.449581174998803710937500000000 \times 10^9$	$-8.64776860916338232383320244317 \times 10^8$
5	$+1.17571125958104512054443359375 \times 10^{13}$	$+1.64145868005800755132947440105 \times 10^{12}$
6	$-3.18064888985252133830423028128 \times 10^{16}$	$-4.16016007587619392285546026342 \times 10^{15}$
7	$+1.03477309951815151989739404812 \times 10^{20}$	$+1.35506144668665011578479155203 \times 10^{19}$
8	$-3.95890060949951787171702519397 \times 10^{23}$	$-5.45740994533040798137376086700 \times 10^{22}$
9	$+1.75802363547448200866475465911 \times 10^{27}$	$+2.63004738948388301397471581365 \times 10^{26}$
10	$-8.98508915233072068697058004551 \times 10^{30}$	$-1.47853891447648836002155944574 \times 10^{30}$
11	$+5.25232959291187236720839982517 \times 10^{34}$	$+9.52631535621939194061435526295 \times 10^{33}$
12	$-3.49297501706658104776470560233 \times 10^{38}$	$-6.95353066637932651872818015613 \times 10^{37}$
13	$+2.62940716668212328895716830967 \times 10^{42}$	$+5.70612739572397688871373383049 \times 10^{41}$
14	$-2.22927146751916684798616723449 \times 10^{46}$	$-5.23539432305661143784168964358 \times 10^{45}$
15	$+2.11808048348488483409151866222 \times 10^{50}$	$+5.34692412323682373417129879084 \times 10^{49}$
20	$-7.67756482076312202465482219049 \times 10^{70}$	$-2.59058872169806959065242368765 \times 10^{70}$
30	$-5.13502619416402678854105232212 \times 10^{114}$	$-2.58371178967762066018120986200 \times 10^{114}$
40	$-1.78804617789836253655584492158 \times 10^{161}$	$-1.19414817113404873895159768413 \times 10^{161}$
50	$-7.33295913933863525514078947399 \times 10^{209}$	$-6.10209745061797542849682305696 \times 10^{209}$
60	$-1.41449923722599152753674938951 \times 10^{260}$	$-1.40914942870226252773832277963 \times 10^{260}$
70	$-6.89053783630996102530832165310 \times 10^{311}$	$-7.99404210639204636195381081171 \times 10^{311}$
75	$+1.39614310998209220877154524815 \times 10^{338}$	$+1.73411445429769522609855678396 \times 10^{338}$

Table 2. Convergence of Padé approximants for energy levels of hydrogen atom in magnetic field. The values taken for comparison from Ref. [21] are marked by *).

γ		0.1		0.4	
	L	$[L/L](\gamma^2)$	$[L/L - 1](\gamma^2)$	$[L/L](\gamma^2)$	$[L/L - 1](\gamma^2)$
$ 1s\rangle$	21	-0.497526480401260	-0.497526480401090	-0.464665	-0.464599
	22	-0.497526480401200	-0.497526480401092	-0.464658	-0.464600
	23	-0.497526480401163	-0.497526480401093	-0.464653	-0.464601
	24	-0.497526480401140	-0.497526480401093	-0.464648	-0.464601
	25	-0.497526480401125	-0.497526480401094	-0.464644	-0.464602
γ		0.16		0.8	
$ 2s\rangle$	21	-0.1236241775347995	-0.1236241775347930	-0.098160	-0.098074
	22	-0.1236241775347966	-0.1236241775347925	-0.098153	-0.098074
	23	-0.1236241775347951	-0.1236241775347928	-0.098147	-0.098077
	24	-0.1236241775347942	-0.1236241775347928	-0.098142	-0.098078
	25	-0.1236241775347937	-0.1236241775347928	-0.098137	-0.098079
		-0.12362418 *)		-0.0980892 *)	
γ		0.27		1.08	
$ 3p\rangle$	21	-0.05468786997811	-0.05468786997805	-0.045436	-0.045412
	22	-0.05468786997796	-0.05468786997784	-0.045430	-0.045398
	23	-0.05468786997795	-0.05468786997790	-0.045428	-0.045404
	24	-0.05468786997793	-0.05468786997788	-0.045425	-0.045402
	25	-0.05468786997791	-0.05468786997789	-0.045423	-0.045404
		-0.05468787 *)		-0.04540638 *)	

Table 3. Coefficients c_i of the power corrections to asymptotics \tilde{E}_k of hydrogen atom hyper-susceptibilities.

<i>state</i>	c_1	c_2	c_3	c_4
$1s$	-2.61829	+1.282	-2.6	-11
$2s$	-8.938	+37.44	-121	$+2.7 \times 10^2$
$2p$	-4.6065	+8.24	-14.3	-4
$3p$	-11.227	+59.5	-239	$+6 \times 10^2$

FIGURE CAPTIONS

Fig. 1. Indices of moments of order k that are related by means of the main recurrence relation. Each of the links A - D represents one of particular cases.

Fig. 2. Summation of the PT series for energy levels with the help of Padé approximants. $E(\gamma) = [25/25](\gamma^2)$ – solid curves, $E(\gamma) = [25/24](\gamma^2)$ – dashed curves. Crosses represent results from Ref. [21].

Fig. 3. Approach of exact hyper-susceptibilities E_k to their asymptotics \tilde{E}_k for the six states of hydrogen atom.

Fig. 4. Calculation of the ground state wave function at the origin $r = 0$ by the moment method. Solid curve was obtained with the help of Padé approximant $[9/9](\gamma^2)$, dashed curve – with the help of $[9/8](\gamma^2)$. Stars denote results of Ref. [23].

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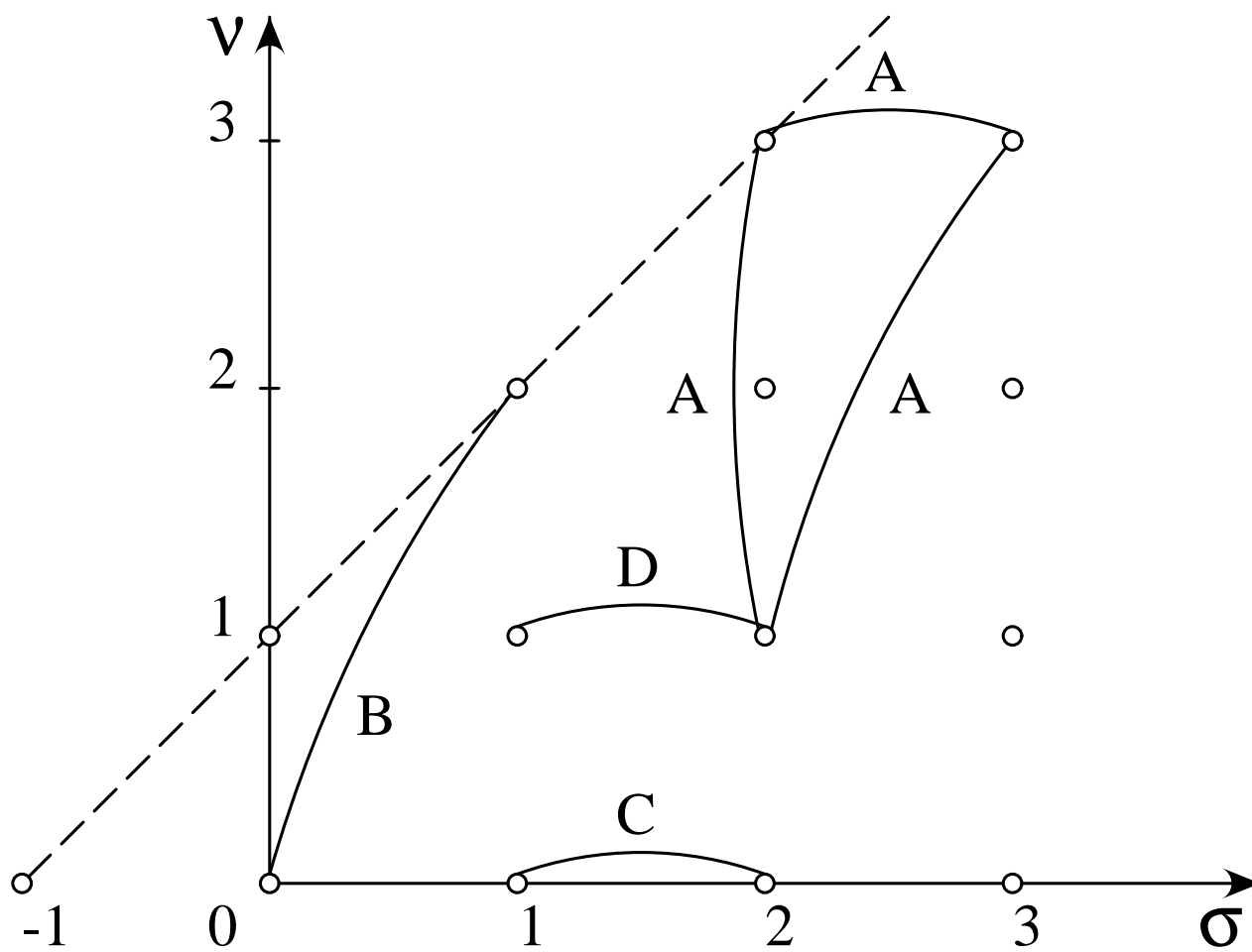


Fig. 1

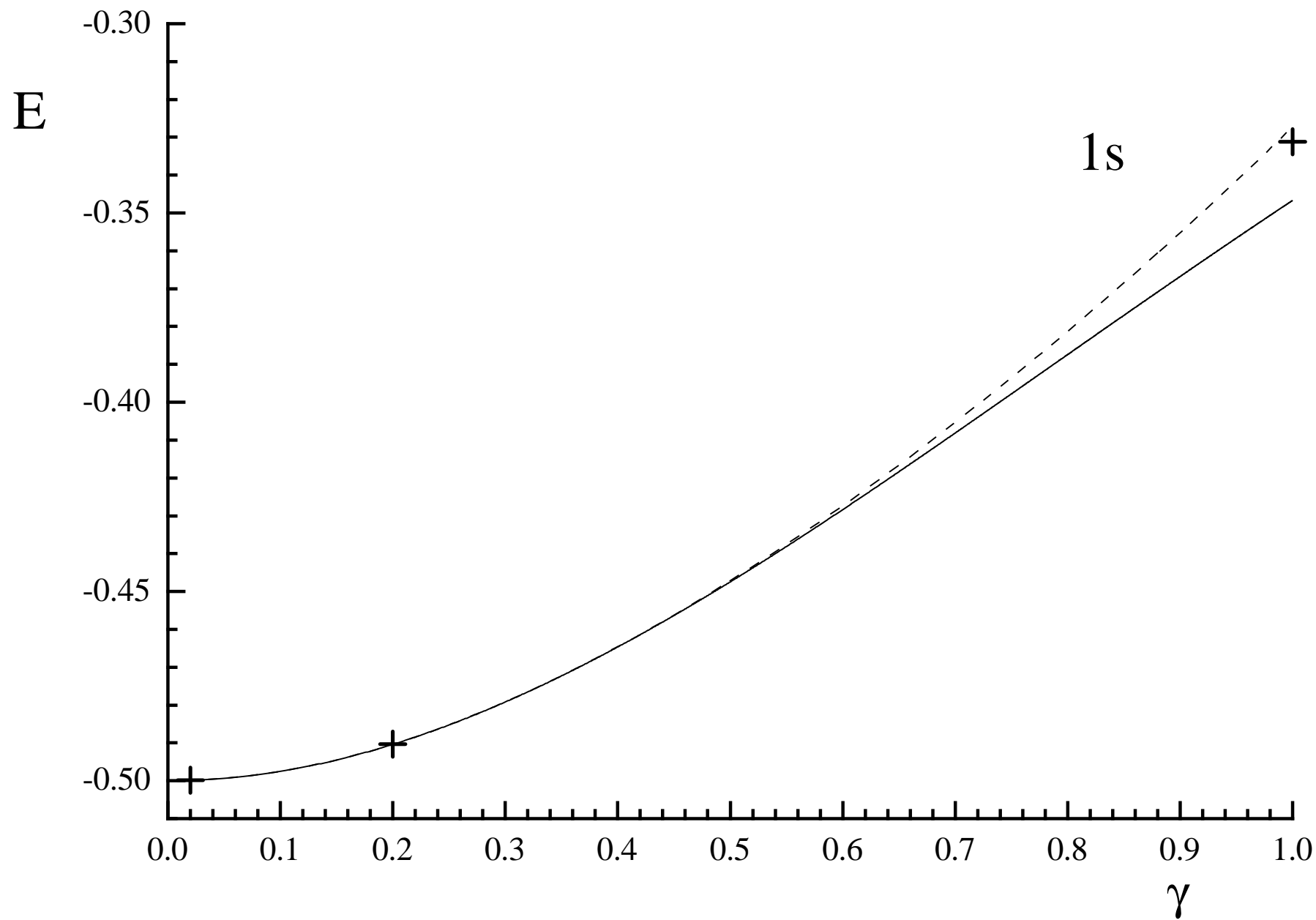


Fig. 2a

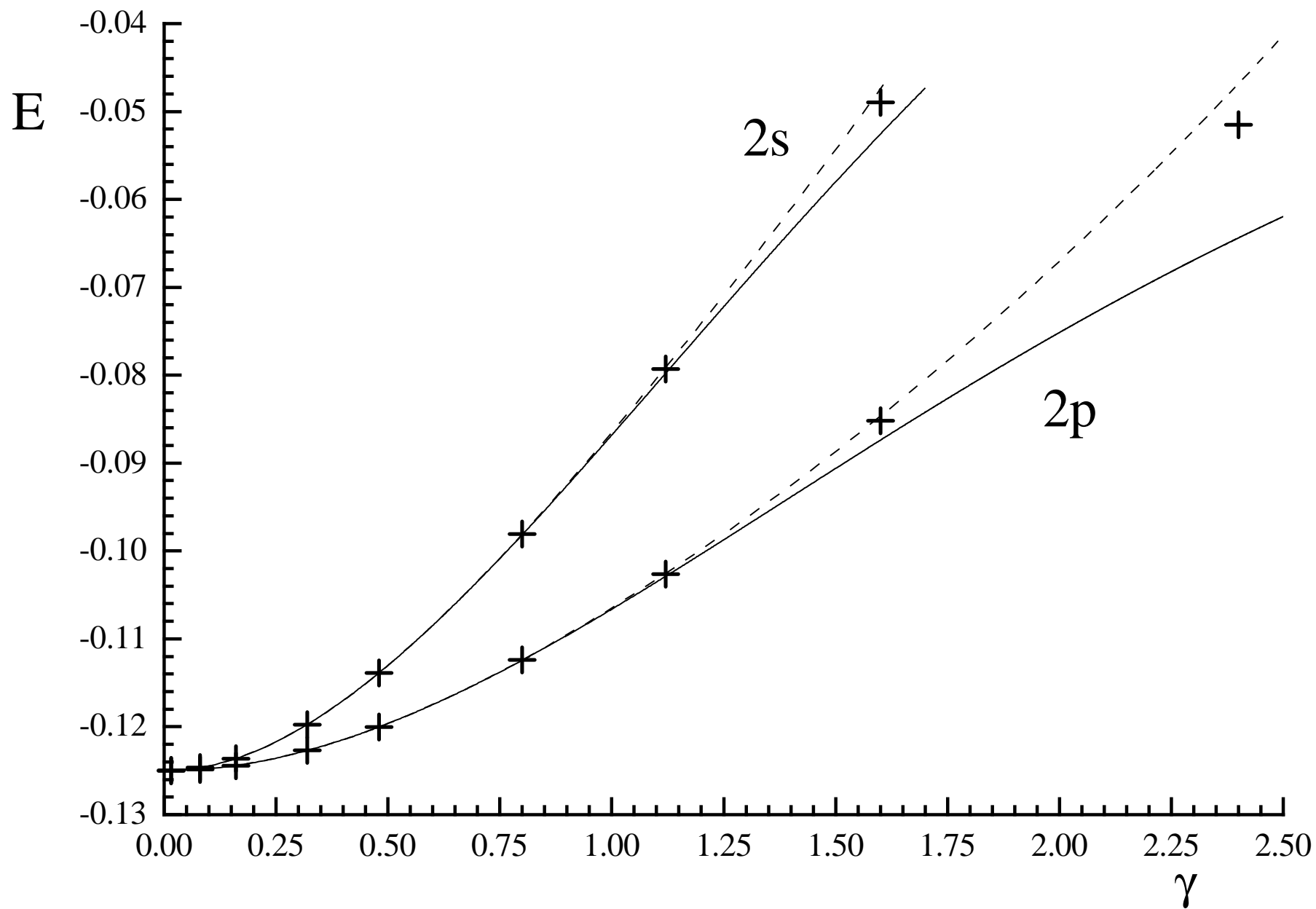


Fig. 2b

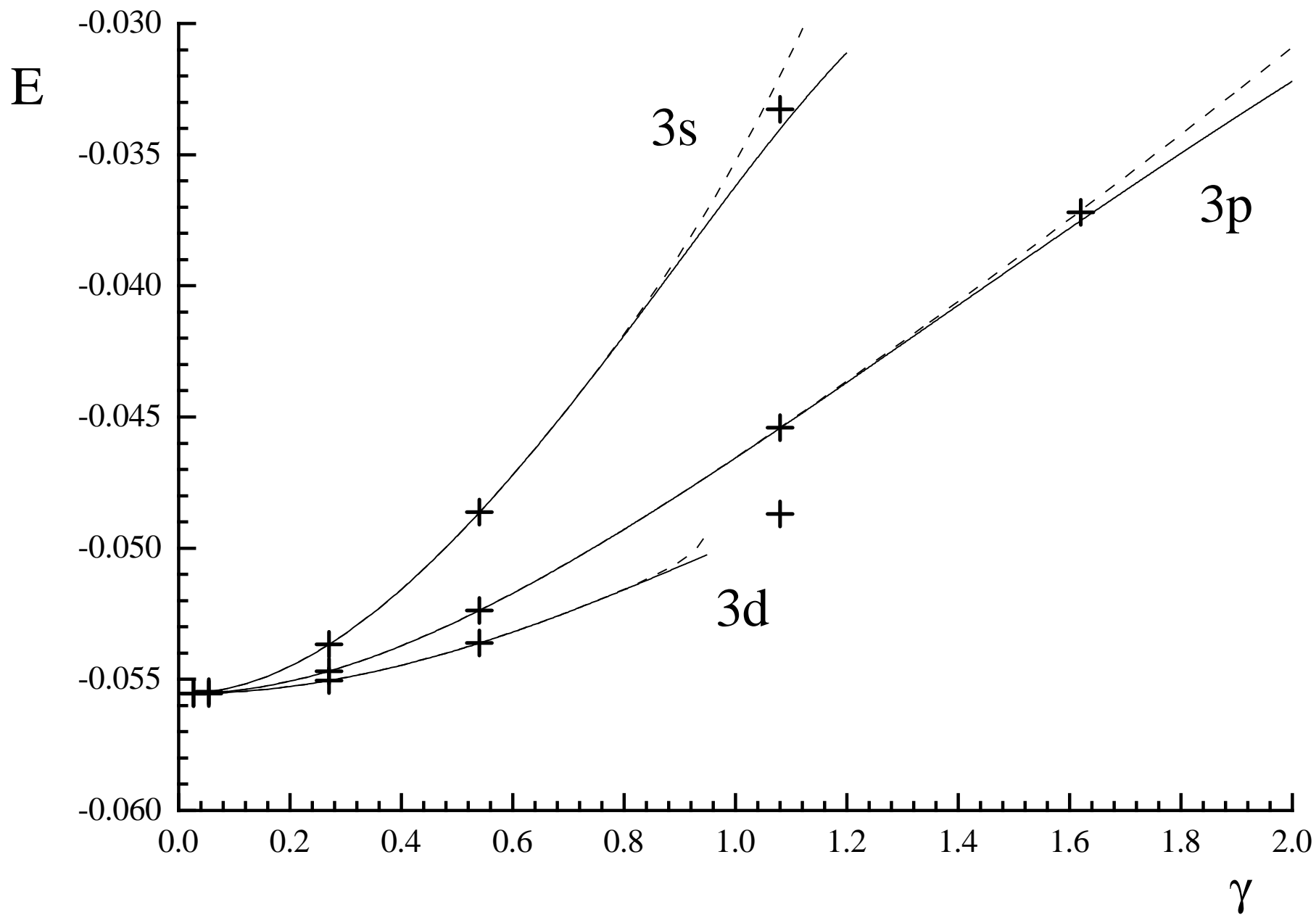


Fig. 2c

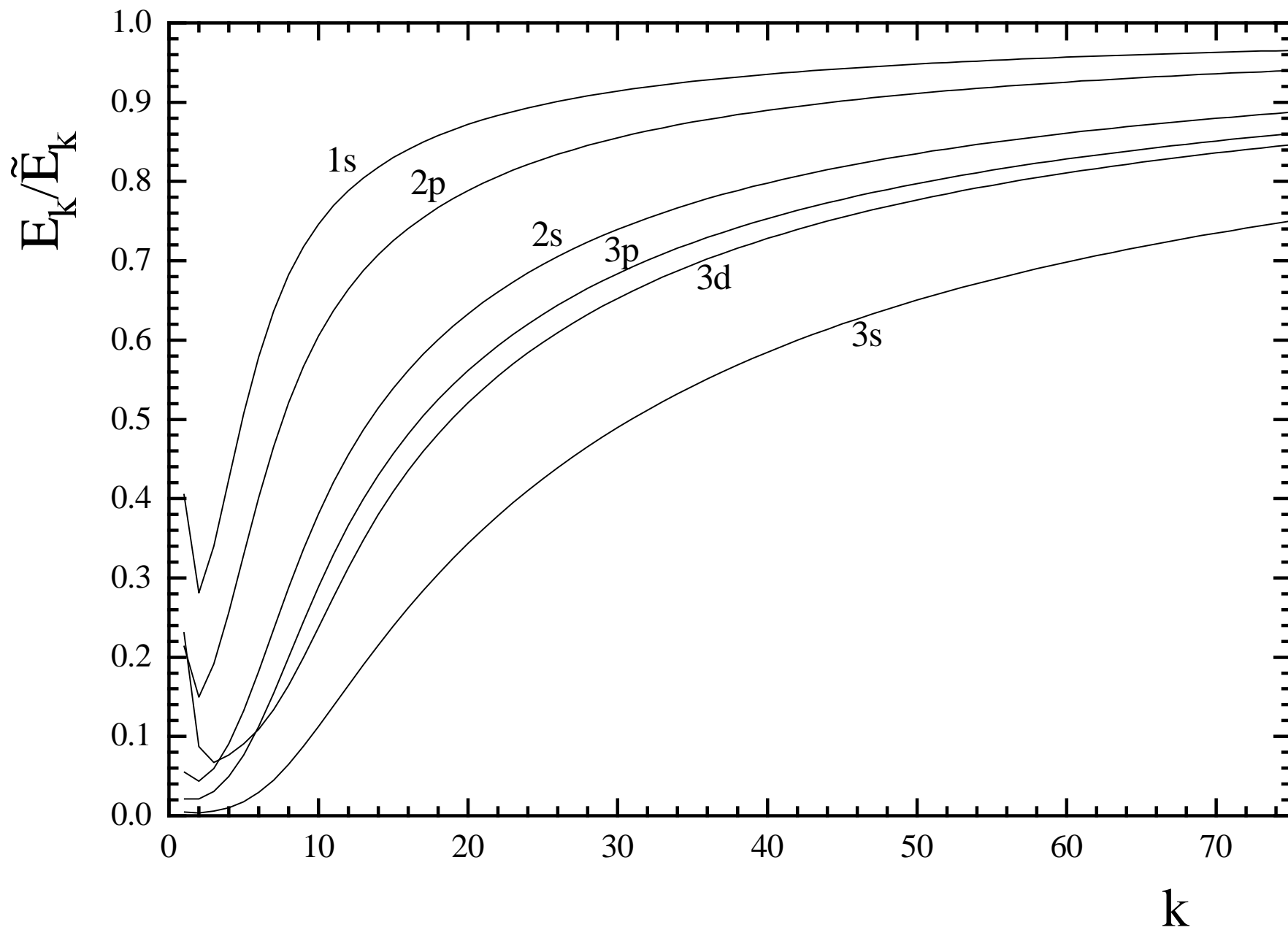


Fig. 3

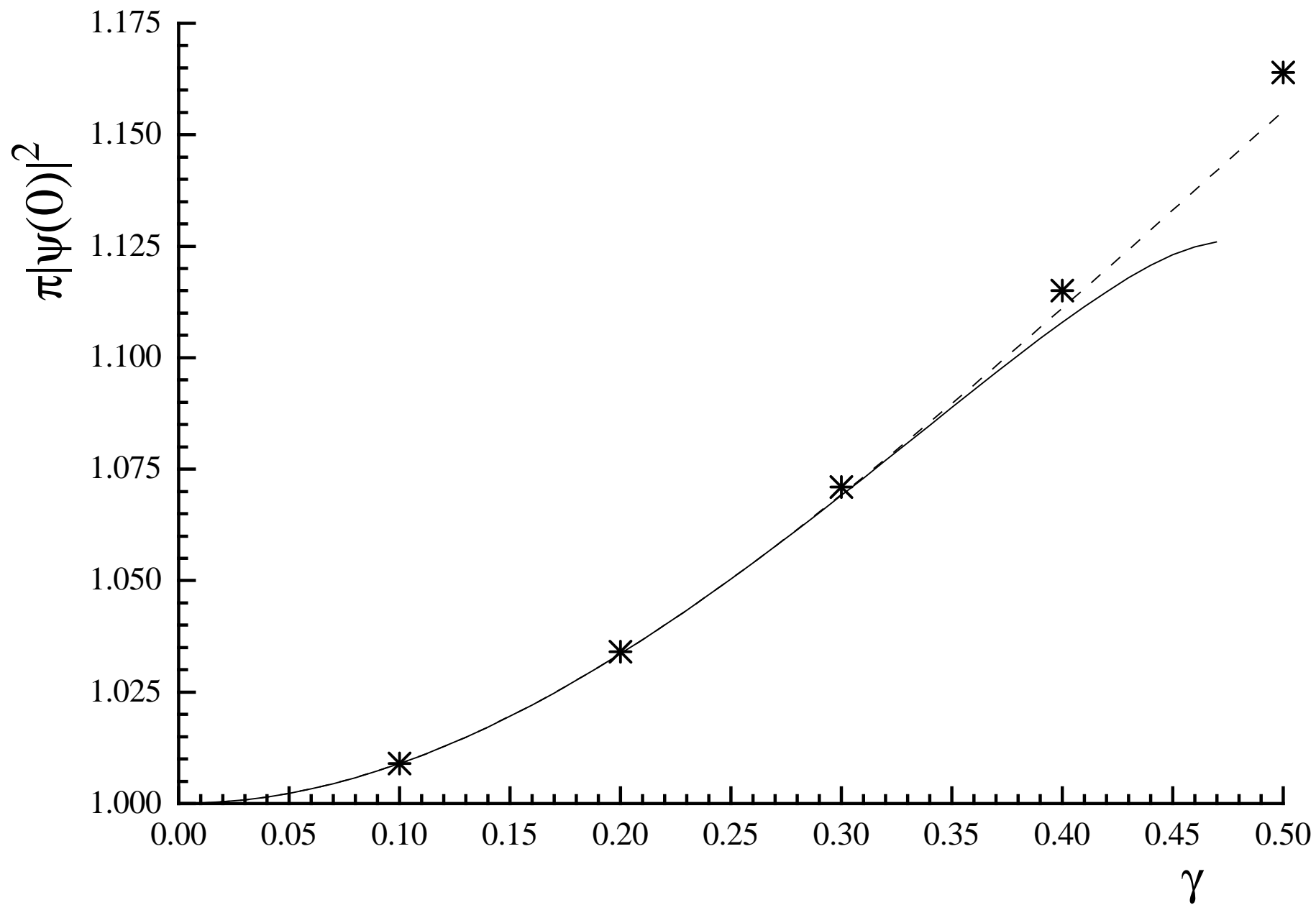


Fig. 4